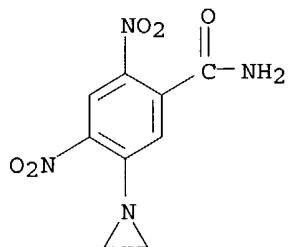


L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 21919-05-1 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN Benzamide, 5-(1-aziridinyl)-2,4-dinitro- (8CI, 9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN 2,4-Dinitro-5-ethyleneiminobenzamide  
 CN 2,4-Dinitroethyleneiminobenzamide  
 CN 5-(1-Aziridinyl)-2,4-dinitrobenzamide  
 CN 5-Aziridino-2,4-dinitrobenzamide  
 CN 5-Aziridinyl-2,4-dinitrobenzamide  
 CN CB 1954  
 CN NSC 115829  
 MF C9 H8 N4 O5  
 LC STN Files: ADISNEWS, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS,  
     BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CHEMCATS, CIN, DDFU, DRUGU,  
     EMBASE, IMSDRUGNEWS, IMSRESEARCH, MEDLINE, PROMT, PROUSDDR, RTECS\*,  
     TOXCENTER, USPAT2, USPATFULL  
     (\*File contains numerically searchable property data)  
 DT.CA CAplus document type: Conference; Dissertation; Journal; Patent  
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);  
     PROC (Process); RACT (Reactant or reagent); USES (Uses)  
 RLD.P Roles for non-specific derivatives from patents: BIOL (Biological  
     study); USES (Uses)  
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological  
     study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP  
     (Properties); RACT (Reactant or reagent); USES (Uses)  
 RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological  
     study); PRP (Properties)

#### Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C2N	NC2	3	C2N	1.28.1	1
C6	C6	6	C6	46.150.18	1



#### Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	5.50	pH 1	(1) ACD
Bioconc. Factor (BCF)	5.50	pH 4	(1) ACD
Bioconc. Factor (BCF)	5.50	pH 7	(1) ACD
Bioconc. Factor (BCF)	5.50	pH 8	(1) ACD

Bioconc. Factor (BCF)	5.50	pH 10	(1) ACD
Boiling Point (BP)	427.2+/-45.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	68.22+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	212.2+/-51.7 deg C		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	2		(1) ACD
Koc (KOC)	118	pH 1	(1) ACD
Koc (KOC)	118	pH 4	(1) ACD
Koc (KOC)	118	pH 7	(1) ACD
Koc (KOC)	118	pH 8	(1) ACD
Koc (KOC)	118	pH 10	(1) ACD
logD (LOGD)	1.28	pH 1	(1) ACD
logD (LOGD)	1.28	pH 4	(1) ACD
logD (LOGD)	1.28	pH 7	(1) ACD
logD (LOGD)	1.28	pH 8	(1) ACD
logD (LOGD)	1.28	pH 10	(1) ACD
logP (LOGP)	1.277+/-0.423		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	252.18		(1) ACD
Vapor Pressure (VP)	1.66E-07 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
 Solaris V4.67 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.  
 153 REFERENCES IN FILE CA (1907 TO DATE)  
 4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 153 REFERENCES IN FILE CAPLUS (1907 TO DATE)

*Scanned*

FILE 'REGISTRY' ENTERED AT 09:28:57 ON 13 JUL 2004

E "5-(AZIRIDIN-1-YL)-2,4-DINITROBENZAMIDE"/CN 25  
E "CB1954"/CN 25  
E "CB 1954"/CN 25

L1 1 S E3

FILE 'CAPLUS' ENTERED AT 09:31:33 ON 13 JUL 2004

L2 151 S 21919-05-1/RN  
L3 3 S L2 AND COSUBSTRATE

FILE 'STNGUIDE' ENTERED AT 09:33:25 ON 13 JUL 2004

FILE 'BIOSIS' ENTERED AT 09:42:13 ON 13 JUL 2004

L4 24 S CB 1954/CN  
L5 0 S L4 AND COSUBSTRATE  
L6 0 S L4 AND DIHYDROPYRIDINE  
L7 0 S L4 AND NAH  
L8 0 S L4 AND NRH

FILE 'PCTFULL' ENTERED AT 09:43:44 ON 13 JUL 2004

L9 0 S 21919-05-1/RN  
L10 0 S CB 1954/CN  
L11 44 S CB1954  
L12 3 S L11 AND NRH

## WEST Search History

DATE: Tuesday, July 13, 2004

<u>Hide?</u>	<u>Set Name</u>	<u>Query</u>	<u>Hit Count</u>
<i>DB=PGPB,USPT,EPAB; PLUR=YES; OP=OR</i>			
<input type="checkbox"/>	L13	L11 and nicotinamide	10
<input type="checkbox"/>	L12	L11 not @py>2000	10
<input type="checkbox"/>	L11	L10 and l7	29
<input type="checkbox"/>	L10	CB adj 1954	37
<input type="checkbox"/>	L9	l7 and L8	5
<input type="checkbox"/>	L8	NQO2	21
<input type="checkbox"/>	L7	prodrugs	19530
<input type="checkbox"/>	L6	l5 and l3	3
<input type="checkbox"/>	L5	bioactivation	310
<input type="checkbox"/>	L4	bioactiviation	1
<input type="checkbox"/>	L3	l1 with (analog or derivative)	778
<input type="checkbox"/>	L2	nicotinamide with analogs	255
<input type="checkbox"/>	L1	nicotinamide	6949

END OF SEARCH HISTORY


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**Web** Results 11 - 17 of about 21 for **NRH OR "dihydroneicotinamide riboside OR "nicotinamide riboside** . (0)

### Function GO Term Classification

... **dihydroneicotinamide riboside** quinone reductase activity;  
dihydropterin oxidase activity; ... L-ascorbate transporter activity;  
**nicotinamide** mononucleotide transporter ...  
[contact14.ics.uci.edu/fgofunction\\_class\\_3.html](http://contact14.ics.uci.edu/fgofunction_class_3.html) - 33k -  
Cached - [Similar pages](#)

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#### **Nicotinamide**

Yahoo! Shopping: Compare and Save.  
Top brands, great stores, low price  
[Yahoo.com](http://www.yahoo.com)

### JBC -- Long et al. 277 (48): 46131

... NQO2 uses **dihydroneicotinamide riboside** (NRH) rather than NAD(P)H as ... **NRH** was synthesized by adding 1,000 units of ... l of 10 mM **nicotinamide** mononucleotide (Sigma ...

[See your message here...](#)

[www.jbc.org/cgi/content/full/277/48/46131](http://www.jbc.org/cgi/content/full/277/48/46131) - [Similar pages](#)

### [PDF] Disruption of Dihydroneicotinamide Riboside:Quinone Oxidoreductase ...

File Format: PDF/Adobe Acrobat

... SP4 0JQ, United Kingdom **Dihydroneicotinamide riboside** (NRH):quinone oxi ... **NRH** was synthesized by adding 1,000 units of ... of 10 m M **nicotinamide** mononucleotide (Sigma ...

[www.jbc.org/cgi/reprint/277/48/46131.pdf](http://www.jbc.org/cgi/reprint/277/48/46131.pdf) - Supplemental Result - [Similar pages](#)

### PNAS -- Zhao et al. 94 (5): 1669

... ionization mass spectrometry; NMNH, reduced **nicotinamide** mononucleotide; QR 1 ... and AK Jaiswal Disruption of **Dihydroneicotinamide Riboside**:Quinone Oxidoreductase ...  
[www.pnas.org/cgi/content/full/94/5/1669](http://www.pnas.org/cgi/content/full/94/5/1669) - [Similar pages](#)

### Bioactivation of 5-(aziridin-1-yl)-2,4-dinitrobenzamide (CB 1954) ...

... NQO2 [NAD(P)H quinone oxidoreductase 2], but its activity is normally latent, and a nonbiogenic co-substrate such as **NRH** [**nicotinamide riboside** (reduced)] is ...  
[www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=PubMed&list\\_uids=10945627&dopt=Citation](http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=PubMed&list_uids=10945627&dopt=Citation) - Supplemental Result - [Similar pages](#)

### DISEOME

... M:Receptors, Muscarinic **nicotinamide** histochemistry muscarinic ... derived nondeletion **NRH** detoxified GGGCGGG GSTM1-positive **riboside** gene-environment ...  
[www.snps3d.org/cgi-bin/tg/index.pl?key=1728&type=geneShell](http://www.snps3d.org/cgi-bin/tg/index.pl?key=1728&type=geneShell) - 101k - Supplemental Result - Cached - [Similar pages](#)

### keywords shared by GSTA2 and NQO1 GSTM1 butyl carcinogens oxidant ...

... alleles of the human reduced **nicotinamide** adenine dinucleotide ... H:quinone oxidoreductase 1 (NQO1) and **dihydroneicotinamide riboside** (NRH):quinone oxidoreductase ...  
[www.snps3d.org/cgi-bin/tg/edge.pl?n1=2939&n2=1728](http://www.snps3d.org/cgi-bin/tg/edge.pl?n1=2939&n2=1728) - 56k - Supplemental Result - Cached - [Similar pages](#)

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